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FOR MORE INFORMATION
Ian Robinson, Department of Physics, University of Illinois at Urbana-Champaign
robinson@mrl.uiuc.edu

Structures of Quantum Wires in Gold/Silicon(557)

I. Robinson[1], P. Bennett[2] and F. Himpsel[3]

[1]University of Illinois; [2]Arizona State University; and [3]University of Wisconsin

Scientists working at NSLS beamline X16A have revealed the full three-dimensional structure of nanowires formed by deposition of gold on a stepped silicon surface using surface X-ray diffraction. The result is important because of the unusual band-dispersion properties previously reported for this system. The result is interesting because the gold atoms are neither imaged by STM, nor are involved directly in the electronic states responsible for the metallic behavior of the surface.

Peter Bennett (left) and Ian Robinson standing in front of the X16A beam station at the NSLS.

A "quantum wire" is a one-dimensional wire created by arranging metal atoms that touch each other in an exact straight line. The wave functions describing the electrons present in such a wire are localized in the directions perpendicular to its axis but can form solitons – waves that propagate with little loss of energy and retain their shape and speed after colliding other such waves – in the direction along the wire. The Pauli exclusion principle forbids the free propagation of these solitons along the wire and leads to a one-dimensional metal with highly unusual properties.

We have investigated a quantum wire in a candidate system for spin-charge separation, due to the formation of a Luttinger liquid, in which electrons have long-range interactions between them.

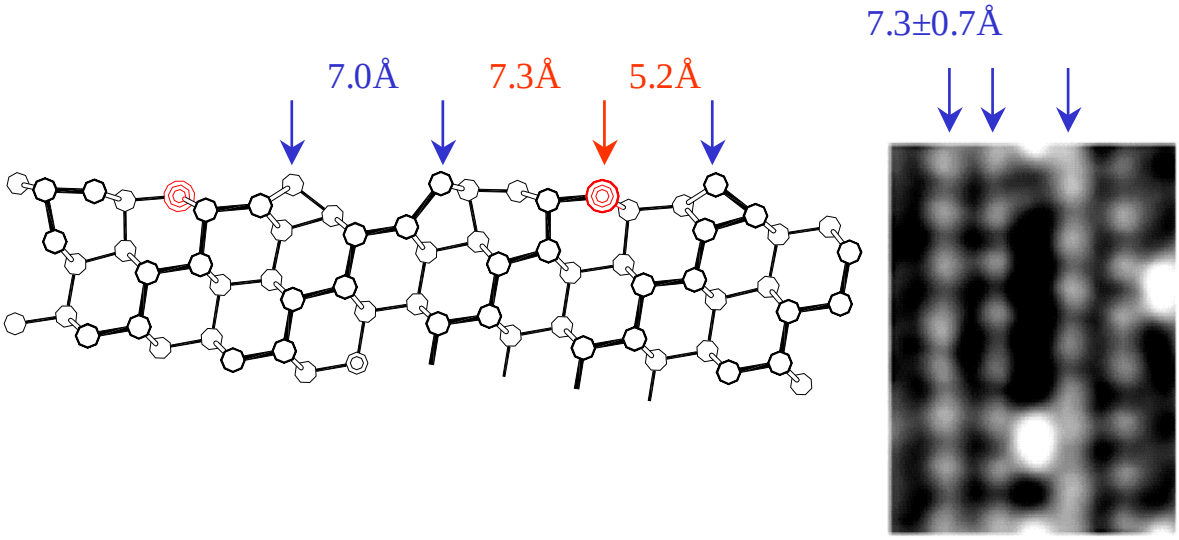
We used two techniques. The first is the scanning tunneling microscope (STM), which uses electron tunneling to map the positions of individual atoms and defects in a surface. Typical defects are vacancies, steps and kinks. We also used surface x-ray diffraction, a traditional structure-determining method that is less useful for looking at defects, but provides accurate three-dimensional structures.

We measured a large set of crystal truncation rods to solve a crystalline structure formed by evaporation of 20 percent of a monolayer of gold onto a silicon(557) surface using the surface x-ray diffraction facility at NSLS beamline X16A.

The derived structure, shown in the figure, reveals four main features. First, the row of gold atoms sits in the middle of the terrace between adjacent steps in the substrate, while we expected that the metal would have directly lined the step edge instead. Second, an almost ideal substitution takes place in the upper bilayer, resulting in bond lengths between gold and silicon of 2.47 angstrom and 2.35 angstrom, which are indistinguishable from the bond length between two silicon atoms, which is 2.35 angstrom. A gold atom appears to substitute in the silicon lattice with relatively little strain. The third feature is that the step edge reconstructs to form a five-membered ring, but removes a dangling bond. Finally, the figure shows a row of adatoms attached to dangling bonds.

The STM micrograph reveals two lines per unit cell that might be mistaken for wires. The X-ray structure has only a single gold per unit cell. Analysis of the inter-row

distances shows that neither of the rows can be gold atoms, which are therefore not visible to STM. The rows correspond instead to the step-edge silicon and the adatom silicon features. Because STM is surface-sensitive, it detects only the outermost electron shells of the topmost layer, whereas surface x-ray diffraction sees the full three-dimensional arrangement of the atom cores.



(Left) Side view of the three dimensional structure of gold nanowires grown on a silicon(557) surface. (Right) The STM image shows two rows of atoms, neither of which corresponds to the single gold atom in the unit cell structure.